

Course Title	Structure of Materials
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Discipline	Materials Science and Engineering
Format	Video

ASSIGNMENTS

Chapter-1: Overview

- 1) From a general perspective what classes of materials exist?
- 2) Based on the arrangement of atoms/molecules/ions, how can we classify materials?
- 3) How can materials be classified based on band structure?
- 4) What is the difference between insulators and semi-conductors?
- 5) What are hybrids and what sub-classes of hybrids exist?
- 6) Give an example of a lattice structure (hybrid type).
- 7) Why do we synthesize hybrids (instead of working with monolithic materials)?
- 8) What are the vertices of a 'materials tetrahedron'?
- 9) How can materials be classified based on bonding?
- 10) What aspects does one need to consider for understanding the properties of materials?
- 11) What common manufacturing methods are employed to fabricate components?
- 12) How can we define microstructure keeping in view the properties?
- 13) How can we 'tailor' the micorstructure?

Chapter-2: Geometry of Crystals

- 1) Based on atomic order, what is the difference between amorphous materials and crystals?
- 2) What are the two ways to define a crystal?
- 3) Define a lattice. How many different types of lattices exist in 2D and 3D?
- 4) What is a motif? Give an example of a motif which will lower the symmetry of a square lattice to give a rectangle crystal.
- 5) What is a primitive unit cell? Why do we use non-primitive unit cells (e.g. for cubic close packed crystal)?
- 6) What are the factors which are taken into account in the choice of the unit cell?
- 7) Which are the seven crystal systems and what are their characteristic symmetries?
- 8) Which is the least symmetry that crystal should have?
- 9) What is the symmetry of a square lattice? What is the symmetry of a face centred cubic (FCC) lattice?
- 10) Analyze the crystal in Figure 1 in terms of sublattices (and 'subcrystals').



Figure 1

- 11) Consider an infinite one dimensional array of points are spaced equally with spacing 'a' (Figure 2). Place an object having the shape of an arrow mark (e.g. \uparrow) at each point to create a crystal of lattice parameter '3a'. Describe this crystal in terms of a Lattice and a Motif. How is the symmetry altered on the formation of a crystal?

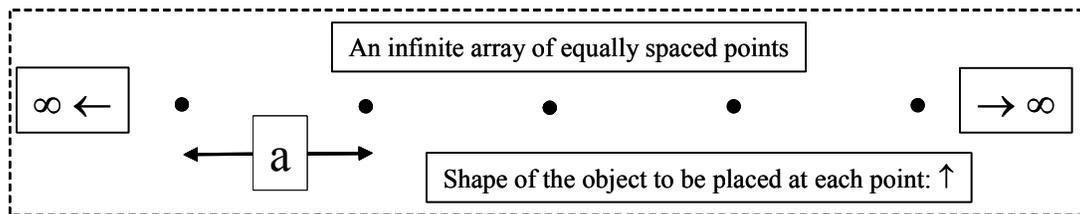


Figure 2

- 12) For the graphene crystal (Figure 3). Mark the lattice points. Draw a unit cell. What is the lattice and the motif?

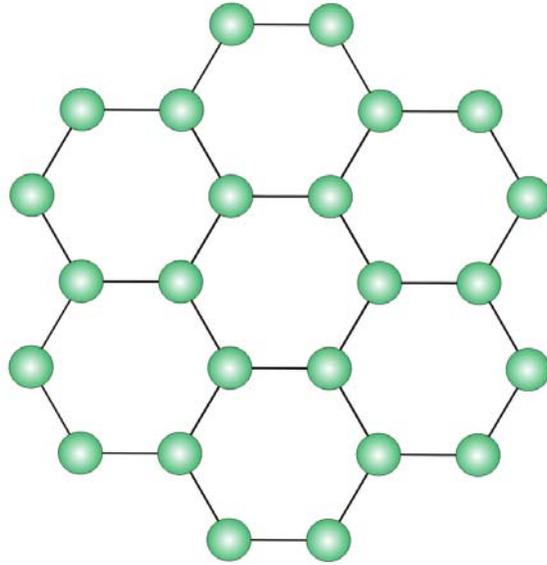


Figure 3

- 13) Why is the C-centred cubic lattice absent? Why is that in hexagonal system, we have only one kind of lattice (the simple one)?
- 14) What is the ratio of volumes for a primitive unit cell to a conventional unit cell for a FCC lattice?

Chapter-3: Miller Indices (including previous topics)

- 1) What does the symbol $[21]$ represent? (Hints: Is it one vector or a set of vectors? What is the start point and the end point? What is its length?).
- 2) Define a family of directions/planes? How is family of planes represented?
- 3) How many members does the $\{111\}$ family have in the copper crystal?
- 4) What is the formula to calculate the interplanar spacing from Miller indices of planes (Cu crystal)?
- 5) What are Miller-Bravais indices used for? Why do we have 4 indices in 3-dimensions in Miller-Bravais indices?
- 6) Draw $(1\bar{1}00)$ and $(2\bar{1}\bar{1}0)$ planes in a hexagonal lattice.
- 7) Miller indices of the intersection of (111) & $(11\bar{1})$ planes in a cubic lattice.
- 8) What is the Weiss zone law? For which crystal systems is this valid?
- 9) With respect to Figure 4:
 - (i) Draw a triply non primitive unit cell (on the figure and label).
 - (ii) Name the crystal: _____.
 - (iii) Overlay the symmetry elements on the figure.
 - (iv) The members of the $\langle 01 \rangle$ family are: _____.
 - (v) The members of the $\langle 11 \rangle$ family are: _____.

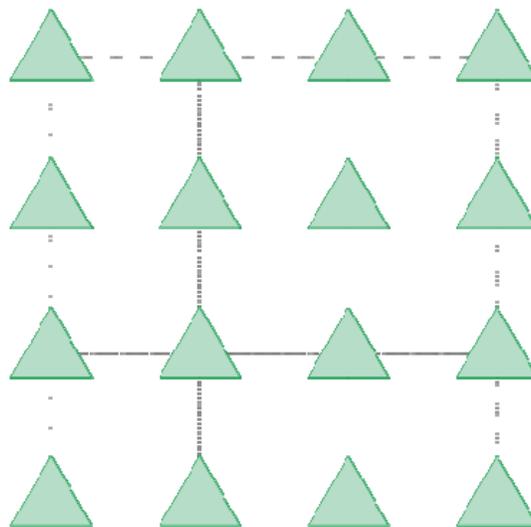


Figure 4

- 10) a) In Figure 5 draw all the symmetry elements (operators)
(Overlay on the figure and do NOT draw the redundant operators).
b) Draw the conventional unit cell and also draw the smallest unit cell.
c) What is the Bravais lattice of the structure? What is the motif?
d) What is the number of lattice points per cell?
e) Draw the fundamental lattice translation vector. What is its Miller index?
(Note: allow for minor drawing/reproducing errors)

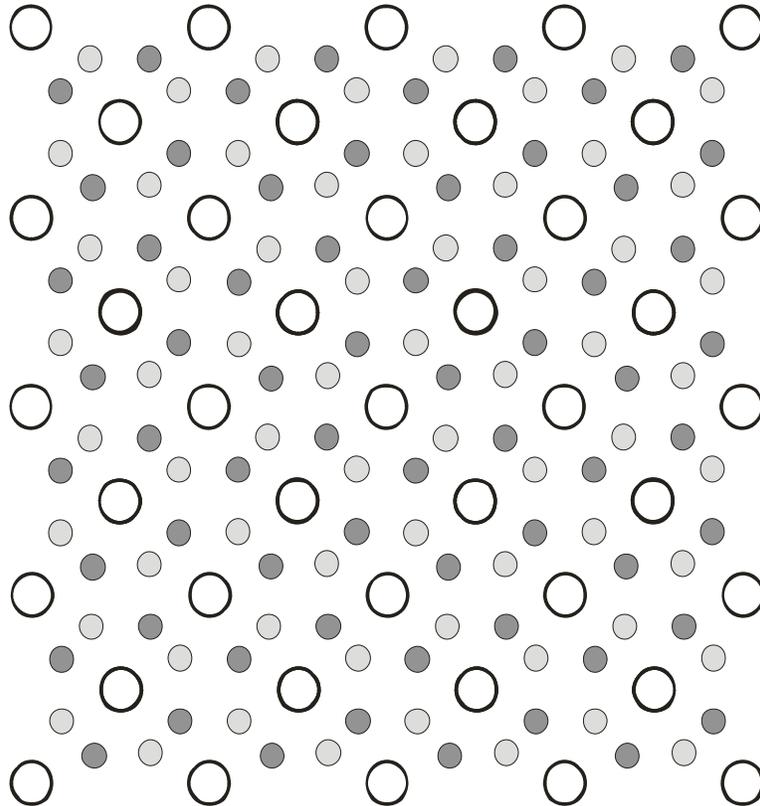


Figure 5

Chapter-4: Crystal Structures

- 1) How is an ideal crystal different from a real crystal? Give examples to show average order of the following types: (i) positional order, (ii) orientational order and (iii) probabilistic occupational order.
- 2) Give common examples of FCC, BCC and HCP metals.
- 3) The following questions pertain to CCP crystals.
 - (a) How can we construct a CCP crystal starting with a layer of close packed atoms?
 - (b) What is the symmetry of the crystal obtained?
 - (c) What is the shape of the coordination polyhedron?
 - (d) What kinds of voids are possible?
 - (e) If the face centre is an octahedral void, the where else is an equivalent position in the unit cell (based on translational symmetry)?
- 4) The following questions pertain to HCP crystals.
 - (a) How can we construct a HCP crystal starting with a layer of close packed atoms? What is the symmetry of this layer?
 - (b) What is the symmetry of the crystal obtained?
 - (c) What is the shape of the coordination polyhedron?
 - (d) What kinds of voids are possible?
 - (e) Describe the structure in terms of a lattice and motif?
- 5) Why are the void types identical across HCP and CCP crystals?
- 6) Calculate the size of the largest atom which can fit in the tetrahedral and octahedral void in a HCP crystal.
- 7) With respect to a BCC crystal:
 - (a) what is the shape of the coordination polyhedron?
 - (b) what are the kinds of voids?
 - (c) what is the packing fraction? (how does it compare with the CCP crystal?)
 - (d) what is the coordination number?
- 8) Draw a unit cell of the NaCl structure. Describe the structure in terms of a lattice and a motif. What is the kind of bonding in the solid? Calculate the packing fraction. Is this a close packed structure?

- 9) Draw a unit cell of the diamond cubic structure. Describe the structure in terms of a lattice and a motif. What is the kind of bonding in diamond crystal? Calculate the packing fraction. Does the structure have a 4-fold rotation axis? If not why is then called a cubic crystal?
- 10) Compute the atomic density of (100), (110) and (111) planes in SC, BCC, FCC crystals. Include only those atoms whose centre of mass lies on the plane.
- 11) In steel carbon is present in the interstitial voids of the BCC Fe crystal. Which void is it present and why? Why is the solubility of C in BCC Fe very limited? How come FCC Fe has more solubility for C (in spite of being a close packed structure)?
- 12) When an alloying element is added to host metal, what are the possibilities?
- 13) State the Hume-Rothery rules. Based on the rules determine which of these two alloys will form an extended solid solution: (i) Ag-Au, (ii) Au-Si.
- 14) Give three examples of ordered structures. What is the symmetry change on ordering?
- 15) Elucidate the principles behind the structure of ionic solids. Explain the structure of NaCl, given that: $r_{\text{Na}^+}/r_{\text{Cl}^-} = (0.97 \text{ \AA})/(1.81 \text{ \AA}) = 0.54$.
- 16) In ZnS, $r_c/r_a = 0.48$, which predicts Octahedral coordination. However, tetrahedral coordination is observed in ZnS, Why?
- 17) List the allotropes of carbon. What is the hybridization characteristics in these forms of carbon?
- 18) Diamond is used for cutting hard materials, while graphite is used as a lubricant. Explain this disparity based on the bonding and structure of these forms of carbon.

Chapter-5: Defects in Crystals

- 1) Give examples of structure sensitive and structure insensitive properties. What is the 'structure' being referred to?
- 2) What does the term 'defect structure' encompass?
- 3) List the ways in which defects in crystals can be classified.
- 4) "Magnetic domain wall is a 'defected region' in a material"— explain the perspective used in this description.
- 5) What are point defects? How are they different from mathematical points?
- 6) Differentiate thermal vacancies and structural vacancies. What are vacancy ordered phases? Thermodynamically analyze the ordering process.
- 7) Explain the phrase: "vacancies are thermodynamically stable defects". Can dislocations be thermodynamically stable?
- 8) List and diagrammatically show the simple point defects in ionic crystals. Give examples of point defects in ionic crystals, which arise from off-stoichiometry.
- 9) What is the equilibrium concentration of vacancies at 800K in Cu. (Data for Cu: Melting point = 1083 °C = 1356K, ΔH_f (Cu vacancy) = 120×10^3 J/mole, k (Boltzmann constant) = 1.38×10^{-23} J/K, R (Gas constant) = 8.314 J/mole/K).
- 10) If a copper rod is heated from 0K to 1250K increases in length by ~2%. What fraction of this increase in length is due to the formation of vacancies? (Use data presented before).
- 11) Explain the role of dislocations in diverse (material) contexts.
- 12) List the different mechanisms of plastic deformation and the importance of slip therein.
- 13) Why is the experimentally measured shear stress for plastic deformation orders of magnitude lower than the theoretical shear strength of crystals.
- 14) Explain how the Burgers circuit is drawn to determine the Burgers vector (**b**).
- 15) Keeping **t**, **b**, slip direction and the process by which the dislocation can leave the slip plane, compare edge and screw dislocations.
- 16) On Figure 6 mark the 'character' of the dislocation in various points/segments.

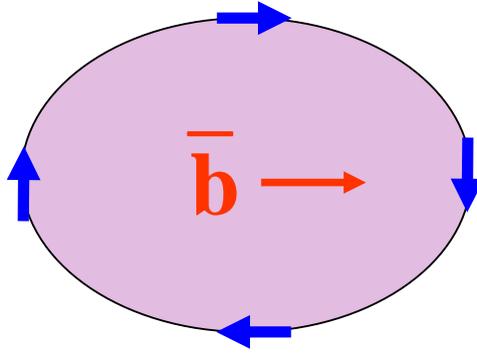


Figure 6

- 17) Where can a dislocation line end?
- 18) Why does a perfect dislocation tend to split into partials? In close packed structures, what is the role of stacking fault energy in this context?
- 19) Draw the σ_{xx} iso-stress contours around an edge dislocation. What is the formula to calculate the elastic energy associated with an edge dislocation (approximately). What is the core of the dislocation in this context?
- 20) What is meant by a slip system? List slip systems in BCC, FCC and HCP crystals.
- 21) Draw and label the following within a unit cell in a CCP structure: (i) slip plane, (ii) \mathbf{b} , (iii) extra half-plane, (iv) line vector.
- 22) What is the Burgers vector in CsCl and NaCl structures?
- 23) How do dislocations arise in crystals? What is the typical dislocation density in an annealed crystal and a cold-worked crystal?
- 24) Define jog and kinks (dislocation line). How can these arise due to dislocation intersection reactions?
- 25) What is the origin of yield point phenomenon observed during tensile testing of steel?
- 26) For a precipitate in the path of a moving dislocation, what is the difference between a coherent and an incoherent precipitate (in terms of the mechanisms operative)?
- 27) What is the origin of image forces? What is the role of dislocations in crystal growth?
- 28) In a cubic crystal a dislocation line of mixed character lies along the $[112]$ direction. Burgers vector = $\frac{1}{2}[110]$. What are the edge and screw components of the Burgers vector? Which is the slip plane?

- 29) In a CCP crystal is the following dislocation reaction feasible energetically:
 $\frac{1}{2}[110] \rightarrow \frac{1}{6}[2\bar{1}\bar{1}] + \frac{1}{6}[121]$? What is the significance of the vectors on the RHS of the reaction?
- 30) Give an overview of homophase and heterophase boundaries.
- 31) Define coherent, semi-coherent and incoherent interfaces. How can we structurally understand semi-coherent interfaces?
- 32) What is the difference between surface energy and surface tension? What are the key differences between solid and liquid surfaces?
- 33) In what kind of solids can we have polar surfaces? Give an example of a polar and a non-polar surface in NaCl. What are the two kinds of (111) surfaces possible in NaCl?
- 34) Conceptually, two surfaces can be made by cutting an infinite solid with a plane. What can happen to the surfaces after the cut?
- 35) Draw schematics to explain the terrace, ledge, kink model of a surface.
- 36) Explain the Wulff construction to determine the equilibrium shape of a crystal.
- 37) What are the macroscopic and microscopic degrees of freedom associated with a grain boundary (created by rotation of one part of the crystal with respect to the other).
- 38) How can we visualize the structure of low angle twist and tilt boundaries.
- 39) Draw a schematic of a semi-coherent epitaxial interface.
- 40) Label the features in the micrograph shown in Figure 7.



Figure 7

Chapter-6: Diffusion in Solids

- 1) What are the roles of diffusion in materials (in various contexts)?
- 2) Explain the Kirkendall effect? What drives diffusion of atoms?
- 3) State the Fick's first law (equation) and explain the terms.
- 4) What is meant by 'Steady and non-steady state diffusion'?
- 5) State the Fick's second law (equation) and write the error function solution to the same.
- 6) Explain the interstitial and vacancy mechanisms of diffusion. Why is interstitial diffusion typically faster (at a given T)?
- 7) List the paths of diffusion with Lesser Resistance than lattice diffusion. Order these in terms of the activation energy for diffusion.
- 8) A 0.2% carbon steel needs to be surface carburized such that the concentration of carbon at 0.2mm depth is 1%. The carburizing medium imposes a surface concentration of carbon of 1.4% and the process is carried out at 900°C (where, Fe is in FCC form). (Data: $D_0(\text{C in } \gamma\text{-Fe}) = 0.7 \times 10^{-4} \text{ m}^2 / \text{s}$, $Q = 157 \text{ kJ / mole}$)
- 9) Derive and approximate formula for the depth of penetration after time 't'.

Chapter-7: Phase Diagrams

- 1) What kinds of phase diagrams are possible? What are the axes in a typical metallurgical phase diagram? What can be the components?
- 2) What kinds of phases exist based on state, atomic order, band structure, property, stability and size/geometry of the entity?
- 3) Explain the term 'equilibrium phase diagrams', in the context of materials phase diagrams.
- 4) State the Gibbs phase rule.
- 5) The following pertain to Figure 8.
 - (a) Compute the degrees of freedom for points/lines/regions marked with dashed ellipses. What are these degrees of freedom?
 - (b) What is the maximum number of phases, which can co-exist in this unary diagram?
 - (c) Why are some lines sloping downward, while others are sloping upward?

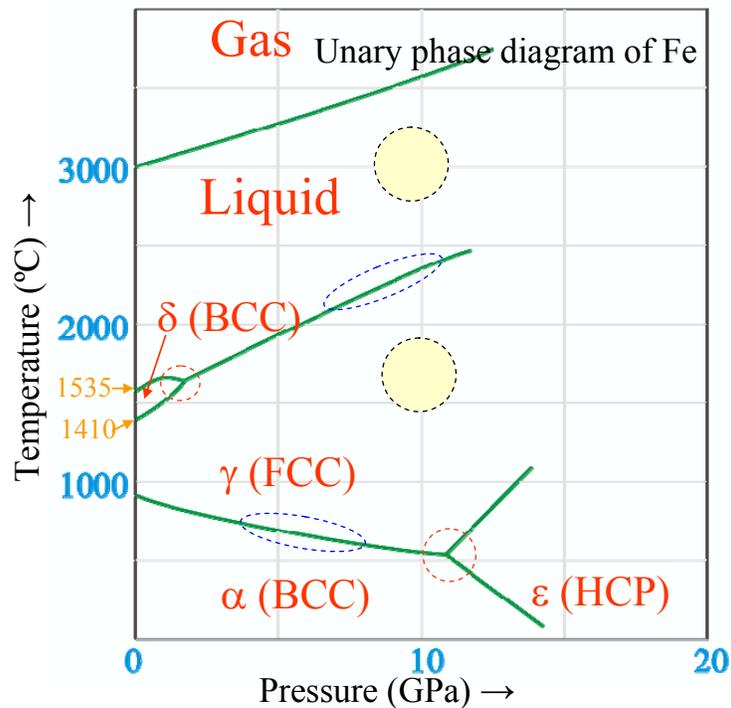


Figure 8

- 6) Classify possible binary phase diagram based on solubility in the liquid and solid states.
- 7) Draw a schematic isomorphous phase diagram. When do we expect two components to form an isomorphous system? Plot the Gibbs free energy versus composition at various

representative temperatures. With respect to Figure 9, calculate the fraction of liquid and solid at T_0 (hint; lever rule).

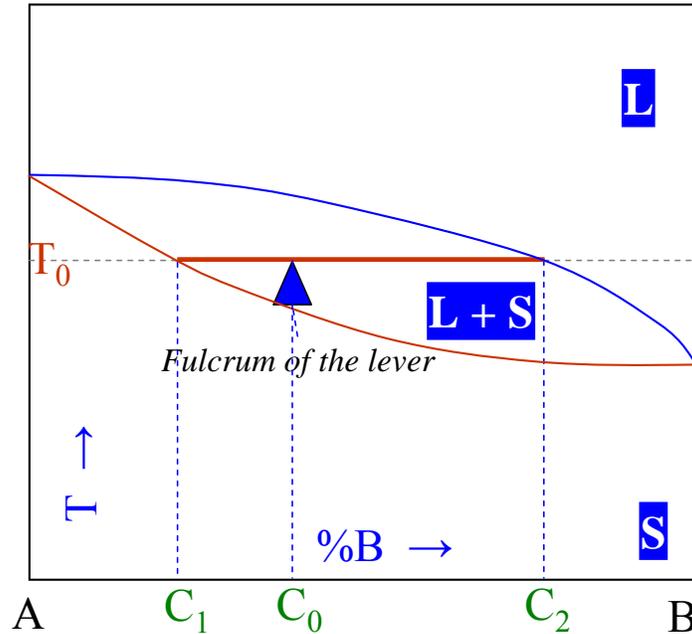


Figure 9

- 8) What are congruently melting alloys in the context of variations to the model isomorphous system? Draw schematics showing ordering and phase separation at 'low' temperatures.
- 9) Draw an illustrative eutectic phase diagram and write down the eutectic reaction (with respect to the figure). What is a typical microstructure obtained, when a eutectic composition is slowly cooled?
- 10) During the solidification of an off eutectic composition (C_0), 90 vol.% of the solid consisted of the eutectic mixture and 10 vol.% of the proeutectic β phase. What is the value of C_0 . (Density data for β and α : $\rho_\alpha = 10300 \text{ Kg/m}^3$, $\rho_\beta = 7300 \text{ Kg/m}^3$). (Eutectic Data: 183°C , 62 wt.% Sn). (Eutectic reaction: $L \xrightarrow[183^\circ\text{C}]{\text{Cool}} \alpha + \beta$ 62%Sn 18%Sn + 97%Sn).
- 11) Draw the iron-cementite phase diagram and list the phase reactions therein. What is pearlite?

Chapter-8: Phase Transformations

- 1) Explain the term microstructural transformations.
- 2) What are the stimuli which one can employ to cause a phase transformation to occur?
- 3) If a part of the volume of material transforms to another phase (all in solid state), this results in a strained state of the material. Explain how.
- 4) What is meant by undercooling?
- 5) Explain how nucleation and growth can lead to a phase transformation.
- 6) Compute critical radius of nuclei r^* and the critical value of ΔG .
- 7) Draw schematic nucleation rate, growth rate and transformation rate curves with increasing undercooling.
- 8) Figure 10 shows a schematic TTT diagram. The transformation from α to β is feasible only below T_m . Why is the transformation sluggish at low and high undercoolings.

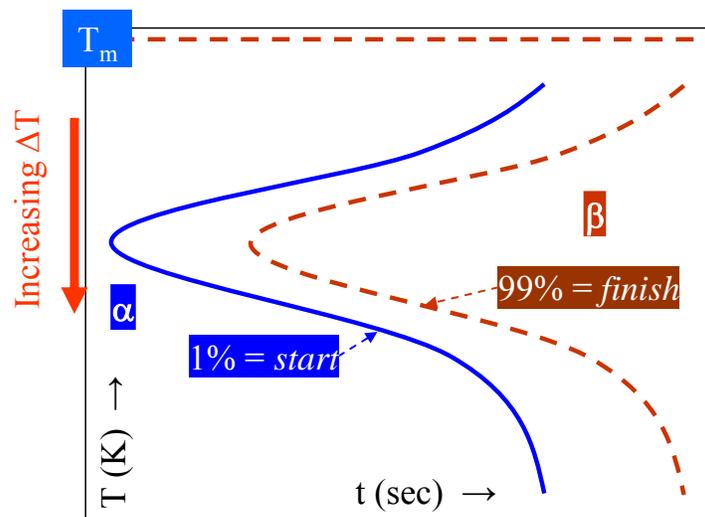


Figure 10

- 9) Draw the TTT diagram for eutectoid steel. What microstructures are obtained if the transformation is carried out above, below and at the nose of the 'C' curve? How will the diagram be altered for hypereutectoid steel?
- 10) Draw the CCT curves for eutectoid steel. What microstructure will be obtained for the following operations: Full Anneal (furnace cooling), Normalizing (Air cooling), Oil Quench and Water Quench. Overlay these cooling curves on the CCT diagram.

- 11) Explain Bain distortion in the context of martensitic transformations. What crystal structure will be produced by the martensitic transformation of pure Fe.
- 12) Why does the hardness of water quenched steel increase as a function of the carbon content in steel?
- 13) Explain recrystallization annealing and stress-relief annealing in the context of steel. What is the role of normalization?
- 14) What is meant by Hardenability? Explain the Jominy End Quench Test to determine Hardenability.
- 15) What is the importance of the tempering operation (after quenching)?
- 16) What is the role of various alloying elements in steel? How do alloying elements increase the hardenability of steel?
- 17) Explain the steps involved in the precipitation hardening of an Al-4wt.% Cu alloy. Draw the hardness versus aging time curve. Why does this plot have a maximum?
- 18) What are GP zones? In low temperature aging why do we get GP zones instead of the stable θ -Al₂Cu phase?
- 19) What is meant by coarsening? Explain the role Gibbs-Thompson effect in this context.
- 20) What is meant by a glass transition? Draw a schematic V-T plot on cooling to show the glass transition.